

Douglas E Spearot

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

83

papers

1,938

citations

23

h-index

41

g-index

87

ext. papers

2,208

ext. citations

4

avg, IF

5.46

L-index

#	Paper	IF	Citations
83	Tensile strength of <1 0 0> and <1 1 0> tilt bicrystal copper interfaces. <i>Acta Materialia</i> , 2007 , 55, 705-714	8.4	192
82	Nucleation of dislocations from [001] bicrystal interfaces in aluminum. <i>Acta Materialia</i> , 2005 , 53, 3579-3589	5.8	177
81	Dislocation nucleation from bicrystal interfaces with dissociated structure. <i>International Journal of Plasticity</i> , 2007 , 23, 143-160	7.6	139
80	Dislocation nucleation from bicrystal interfaces and grain boundary ledges: Relationship to nanocrystalline deformation. <i>Journal of the Mechanics and Physics of Solids</i> , 2007 , 55, 2300-2327	5	104
79	Atomistic simulations of homogeneous dislocation nucleation in single crystal copper. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2007 , 15, 693-709	2	104
78	Two-dimensional MoS ₂ under ion irradiation: from controlled defect production to electronic structure engineering. <i>2D Materials</i> , 2017 , 4, 025078	5.9	99
77	Insights on slip transmission at grain boundaries from atomistic simulations. <i>Current Opinion in Solid State and Materials Science</i> , 2014 , 18, 188-195	12	77
76	Non-local separation constitutive laws for interfaces and their relation to nanoscale simulations. <i>Mechanics of Materials</i> , 2004 , 36, 825-847	3.3	75
75	Fracture mechanics of monolayer molybdenum disulfide. <i>Nanotechnology</i> , 2015 , 26, 175703	3.4	59
74	Effect of point and grain boundary defects on the mechanical behavior of monolayer MoS ₂ under tension via atomistic simulations. <i>Journal of Applied Physics</i> , 2014 , 116, 013508	2.5	54
73	Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals. <i>Dislocations in Solids</i> , 2008 , 14, 43-139		46
72	Atomistic Modeling of Grain Boundaries and Dislocation Processes in Metallic Polycrystalline Materials. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , 2009 , 131,	1.8	35
71	Phase transformation in monolayer molybdenum disulphide (MoS ₂) under tension predicted by molecular dynamics simulations. <i>Scripta Materialia</i> , 2014 , 76, 41-44	5.6	32
70	Traction-separation relationships for hydrogen induced grain boundary embrittlement in nickel via molecular dynamics simulations. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2016 , 650, 354-364	5.3	29
69	A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations. <i>Jom</i> , 2014 , 66, 408-416	2.1	29
68	Evolution of the E structural unit during uniaxial and constrained tensile deformation. <i>Mechanics Research Communications</i> , 2008 , 35, 81-88	2.2	29
67	Plastic deformation of nanocrystalline copper-antimony alloys. <i>Journal of Materials Research</i> , 2010 , 25, 411-421	2.5	27

66	Visco-hyperelastic constitutive modeling of strain rate sensitive soft materials. <i>Journal of the Mechanics and Physics of Solids</i> , 2020 , 135, 103777	5	27
65	A molecular dynamics study of dislocation density generation and plastic relaxation during shock of single crystal Cu. <i>Journal of Applied Physics</i> , 2016 , 120, 045902	2.5	27
64	On the elastic tensile deformation of <100> bicrystal interfaces in copper. <i>Computational Materials Science</i> , 2008 , 42, 57-67	3.2	26
63	Microstructural stability of copper with antimony dopants at grain boundaries: experiments and molecular dynamics simulations. <i>Journal of Materials Science</i> , 2010 , 45, 6707-6718	4.3	25
62	Molecular dynamics simulation of nanoconfinement induced organization of n-decane. <i>Langmuir</i> , 2009 , 25, 7553-60	4	24
61	Mobility of dislocations in Aluminum: Faceting and asymmetry during nanoscale dislocation shear loop expansion. <i>Acta Materialia</i> , 2019 , 168, 426-435	8.4	23
60	A molecular dynamics study of the role of grain size and orientation on compression of nanocrystalline Cu during shock. <i>Computational Materials Science</i> , 2015 , 108, 226-232	3.2	22
59	Simultaneous twinning and microband formation under dynamic compression in a high entropy alloy with a complex energetic landscape. <i>Acta Materialia</i> , 2020 , 200, 1-11	8.4	20
58	Effect of deformation path sequence on the behavior of nanoscale copper bicrystal interfaces. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , 2005 , 127, 374-382	1.8	19
57	Hyperelastic constitutive modeling of hydrogels based on primary deformation modes and validation under 3D stress states. <i>International Journal of Engineering Science</i> , 2020 , 154, 103314	5.7	18
56	A primer on selecting grain boundary sets for comparison of interfacial fracture properties in molecular dynamics simulations. <i>Scientific Reports</i> , 2017 , 7, 8332	4.9	18
55	Heterogeneous dislocation nucleation in single crystal copper-antimony solid-solution alloys. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2009 , 17, 055001	2	18
54	Thermodynamics-based stability criteria for constitutive equations of isotropic hyperelastic solids. <i>Journal of the Mechanics and Physics of Solids</i> , 2019 , 124, 115-142	5	16
53	Phase-field simulations of microstructure evolution during physical vapor deposition of single-phase thin films. <i>Computational Materials Science</i> , 2017 , 131, 170-177	3.2	14
52	Nanoscale dislocation shear loops at static equilibrium and finite temperature. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2017 , 25, 085014	2	14
51	The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature. <i>Computational Materials Science</i> , 2014 , 86, 38-42	3.2	14
50	Molecular Dynamics Simulations of Dislocation Activity in Single-Crystal and Nanocrystalline Copper Doped with Antimony. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2010 , 41, 854-860	2.3	14
49	Atomic-level deformation of Cu_xZr_{100-x} metallic glasses under shock loading. <i>Journal of Applied Physics</i> , 2018 , 123, 215101	2.5	14

48	Shock compression of Cu x Zr100x metallic glasses from molecular dynamics simulations. <i>Journal of Materials Science</i> , 2018 , 53, 5719-5732	4.3	13
47	Microstructure stability of nanocrystalline materials using dopants. <i>Molecular Simulation</i> , 2008 , 34, 35-40		12
46	Effect of water concentration on the shock response of polyethylene glycol diacrylate (PEGDA) hydrogels: A molecular dynamics study. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2019 , 90, 30-39	4.1	12
45	Integrating in situ TEM experiments and atomistic simulations for defect mechanics. <i>Current Opinion in Solid State and Materials Science</i> , 2019 , 23, 117-128	12	11
44	Molecular dynamics simulation of diffusion of small atmospheric penetrates in polydimethylsiloxane. <i>Molecular Simulation</i> , 2011 , 37, 115-122	2	11
43	Influence of vacancy defect concentration on the combustion of reactive Ni/Al nanolaminates. <i>Journal of Applied Physics</i> , 2018 , 124, 045105	2.5	10
42	Melting of Ni and Fe nanoparticles: a molecular dynamics study with application to carbon nanotube synthesis. <i>Journal of Nanoscience and Nanotechnology</i> , 2010 , 10, 5587-93	1.3	10
41	Molecular Dynamics Simulations of Diffusion of O2 and N2 Penetrants in Polydimethylsiloxane-Based Nanocomposites. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , 2012 , 134,	1.8	10
40	Shear-driven motion of Mg {101} twin boundaries via disconnection terrace nucleation, growth, and coalescence. <i>Physical Review Materials</i> , 2019 , 3,	3.2	10
39	Fracture mechanics of multi-layer molybdenum disulfide. <i>Engineering Fracture Mechanics</i> , 2019 , 212, 1-12	4.2	9
38	Atomistic simulation and virtual diffraction characterization of homophase and heterophase alumina interfaces. <i>Acta Materialia</i> , 2015 , 82, 403-413	8.4	9
37	Structure and kinetics of three-dimensional defects on the {101} twin boundary in magnesium: Atomistic and phase-field simulations. <i>Mechanics of Materials</i> , 2020 , 143, 103314	3.3	9
36	Mobility of dislocations in aluminum: The role of non-Schmid stress state. <i>Acta Materialia</i> , 2020 , 185, 420-432	8.4	9
35	Phase-field models for simulating physical vapor deposition and grain evolution of isotropic single-phase polycrystalline thin films. <i>Computational Materials Science</i> , 2016 , 123, 111-120	3.2	9
34	Pressure Dependence of the Peierls Stress in Aluminum. <i>Jom</i> , 2018 , 70, 1094-1099	2.1	8
33	Atomistic simulation and virtual diffraction characterization of stable and metastable alumina surfaces. <i>Acta Materialia</i> , 2014 , 78, 354-368	8.4	8
32	Molecular dynamics simulation of O2 diffusion in polydimethylsiloxane (PDMS) and end-linked PDMS networks. <i>Molecular Simulation</i> , 2014 , 40, 976-986	2	8
31	Interatomic potential for copper-antimony in dilute solid-solution alloys and application to single crystal dislocation nucleation. <i>Computational Materials Science</i> , 2009 , 44, 1258-1264	3.2	8

30	Spectrum of embrittling potencies and relation to properties of symmetric-tilt grain boundaries. <i>Acta Materialia</i> , 2021 , 205, 116527	8.4	8
29	Void collapse and subsequent spallation in Cu ₅₀ Zr ₅₀ metallic glass under shock loading by molecular dynamics simulations. <i>Journal of Applied Physics</i> , 2019 , 125, 215903	2.5	7
28	Transient-State Rheological Behavior of Poly(ethylene glycol) Diacrylate Hydrogels at High Shear Strain Rates. <i>Macromolecules</i> , 2019 , 52, 5860-5871	5.5	7
27	Grain size effects on Ni/Al nanolaminate combustion. <i>Journal of Materials Research</i> , 2019 , 34, 2229-2238	2.5	6
26	Role of grain boundary structure on diffusion and dissolution during Ni/Al nanolaminate combustion. <i>Journal of Applied Physics</i> , 2020 , 127, 125111	2.5	6
25	Behavior of dopant-modified interfaces in metallic nanocrystalline materials. <i>Jom</i> , 2010 , 62, 70-74	2.1	6
24	Mechanical properties of stabilized nanocrystalline FCC metals. <i>Journal of Applied Physics</i> , 2019 , 126, 110901	2.5	5
23	Virtual diffraction analysis of dislocations and dislocation networks in discrete dislocation dynamics simulations. <i>Computational Materials Science</i> , 2020 , 174, 109473	3.2	5
22	Mechanical behavior of core-shell nanostructures. <i>Journal of Materials Science</i> , 2020 , 55, 4303-4310	4.3	5
21	Effect of the initial temperature on the shock response of Cu ₅₀ Zr ₅₀ bulk metallic glass by molecular dynamics simulation. <i>Journal of Applied Physics</i> , 2021 , 129, 165103	2.5	5
20	Effect of Loop Defects on the High Strain Rate Behavior of PEGDA Hydrogels: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 2029-2039	3.4	4
19	Zr segregation in Ni ₃ Zr alloy: implication on deformation mechanism during shear loading and bending creep. <i>Journal of Materials Science</i> , 2020 , 55, 6172-6186	4.3	4
18	Bridging atomistic simulations and experiments via virtual diffraction: understanding homophase grain boundary and heterophase interface structures. <i>Journal of Materials Science</i> , 2016 , 51, 1251-1260	4.3	4
17	Performance Improvement and Workflow Development of Virtual Diffraction Calculations 2014 ,		4
16	An embedded-atom method potential parameterized for sulfur-induced embrittlement of nickel. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 085016	2	4
15	Physical vapor deposition of multiphase materials with phase nucleation via a coupled phase-field approach. <i>Computational Materials Science</i> , 2018 , 143, 71-79	3.2	4
14	Molecular dynamics simulation of the shock response of materials: A tutorial. <i>Journal of Applied Physics</i> , 2022 , 131, 051101	2.5	3
13	Mobility of dislocations in FeNiCrCoCu high entropy alloys. <i>Modelling and Simulation in Materials Science and Engineering</i> ,	2	3

12	Simulation of kinematic Kikuchi diffraction patterns from atomistic structures. <i>MethodsX</i> , 2018 , 5, 1187-1203	3	3
11	Validated tensile characterization of the strain rate dependence in soft materials. <i>International Journal of Impact Engineering</i> , 2021 , 156, 103949	4	3
10	Role of equilibrium and non-equilibrium grain boundary stress fields on dislocation transmission. <i>Journal of Materials Research</i> , 2021 , 36, 2687-2704	2.5	2
9	Algorithm Development in Computational Materials Science. <i>Jom</i> , 2014 , 66, 397-398	2.1	1
8	Molecular Dynamics Simulations of Dislocation Nucleation From Bicrystal Interfaces in FCC Metals 2005 , 505		1
7	On shockwave propagation and attenuation in poly(ethylene glycol) diacrylate hydrogels. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2021 , 118, 104423	4.1	1
6	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials 2018 , 1-34		1
5	Disclination-dislocation based model for grain boundary stress field evolution due to slip transmission history and influence on subsequent dislocation transmission. <i>Journal of the Mechanics and Physics of Solids</i> , 2022 , 104920	5	0
4	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials 2019 , 357-390		
3	Foreword: Modeling, Simulation, and Theory of Nanomechanical Materials Behavior. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2011 , 42, 3867-3867	2.3	
2	Role of grain boundaries and substrate in plastic deformation of core-shell nanostructures. <i>Journal of Materials Science</i> , 2020 , 55, 16990-16999	4.3	
1	Data-driven analysis of neutron diffraction line profiles: application to plastically deformed Ta.. <i>Scientific Reports</i> , 2022 , 12, 5628	4.9	